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NUMERICAL SOLUTION OF A GASIFICATION PROBLEM.(U)
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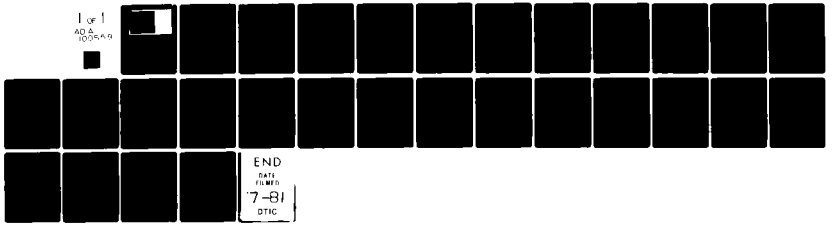

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NUMERICAL SOLUTION OF A GASIFICATION PROBLEM

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ABSTRACT

A problem of gasification and heating of a solid due to the action of an external energy source is discussed. The problem involves a moving boundary when the solid gasifies. At parts of the boundary where gasification is taking place, a model problem looks very much like the one-phase Stefan problem with an energy source at the moving boundary. However, any gas produced is assumed to blow away immediately, and there is no conduction to the solid from the outside, even when the surface temperature of the solid is below the gasification temperature. Accordingly, if the temperature is extended to a function defined over all space by setting it equal to the gasification temperature outside, the temperature will not necessarily be continuous at the boundary, and instead a Neumann condition may be satisfied there. Also, no resolidification is possible, so that the region occupied by the solid cannot increase. Thus, one has the possibility of a situation in which the boundary may alternately move and be stationary. A generalized formulation of the problem is given, a numerical algorithm is described, and computational results are presented.

AMS (MOS) Subject Classifications: 35K50, 35K65, 65C20, 65N05

Key Words: Free boundary problem, Neumann conditions, Gasification, Ablation, Stefan problem

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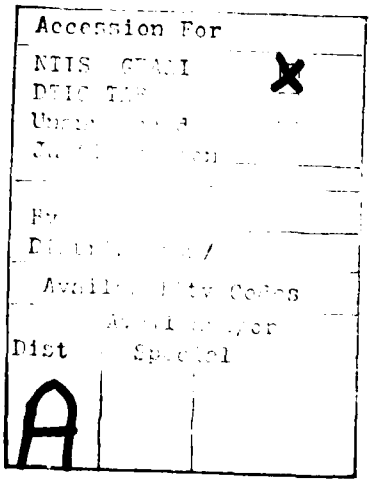
SIGNIFICANCE AND EXPLANATION

The classical Stefan problem models the evolution of the ice-water interface in a melting process as it moves under the influence of heat conduction in the two phases. The gasification problem arises when one irradiates a solid and vaporizes a portion of it, with the gas blowing away. The gasification problem differs from the Stefan problem in that the front can move in only one direction, and the gas cannot resolidify.

In contrast to the case with the Stefan problem, in the gasification problem the solid boundary can stop moving and start cooling down. In that case the nature of the boundary conditions to be satisfied changes. A key goal of this paper is to devise an algorithm which will automatically solve one or the other type of boundary value problem as it becomes the relevant one.

The paper presents an algorithm which solves a variety of boundary value problems without explicitly locating the boundaries in question. Also included is a means of treating the deposition of energy on a surface without location of the surface. Numerical results are obtained and compared with the qualitative properties of solutions previously anticipated.



NUMERICAL SOLUTION OF A GASIFICATION PROBLEM

Joel C. W. Rogers

1. Introduction

The problem we consider is of the following sort: A solid material is exposed to an external source of heat. Heat is conducted internally through the solid, and when the solid reaches a critical temperature, it gasifies. The gas thus formed blows away and no longer interacts with the solid. In the version of the problem given here, the external heat source is radiant energy, to which the solid is opaque and to which the medium external to the solid is transparent. However, other types of heat sources may be treated as well; in particular, heat sources of a frictional nature at the surface of the solid may be considered, in which case the problem is better known as an "ablation" problem.

In the next section we will proceed with a careful description of the phenomena we expect to find associated with the gasification process, and in particular we will analyze the ways in which this problem resembles and differs from the classical Stefan problem. On the basis of this analysis, we will begin development of a mathematical model. A third section will discuss more specifically a time-discretized version of the model, the treatment of boundary conditions, etc. Following this, there will be a brief description of a numerical quadrature of the model, as well as computational results for a particular problem whose initial and boundary data will have been chosen so as to bring about a solution exhibiting the phenomena which are anticipated in the second section. A final section addresses the question of the nature of

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the dependence of solutions of the time-discretized problem on the initial and boundary data. We show that this dependence is not generally monotone in character. Various weakened types of monotonicity which may hold are only conjectured.

We should make it clear that we have not answered the critical question of convergence of the algorithm presented here, nor the questions regarding stability and regularity for the approximate solutions generated by the algorithm. However, we would not have presented this paper unless, bolstered by confidence in the essential correctness of our analysis of the salient features of the gasification problem and the numerical results that we had obtained, we felt that the convergence of the algorithm to a solution of the problem could be proved.

With regard to the mathematical theory of solutions of nonlinear parabolic equations, we place the importance of this problem in the following context. The theory of the classical Stefan problem we consider to be in fairly good shape, in respect both to the basic questions of existence and uniqueness of solutions and of effective computational methods for solution. For systems of degenerate parabolic equations in several space variables, the situation is more complicated: The proofs of monotonicity and stability for solutions of the Stefan problem do not go over to the general case of systems, and indeed for some systems modeling phase transitions with solute diffusion, the experimental evidence and some linear perturbation theories point to a high degree of instability and complexity for the boundaries between different phases [7]. The difficulties arising in the treatment of parabolic systems in several space variables are in some respects similar to those encountered in the study of hyperbolic systems in several space variables [5]. The gasification problem belongs to what may be the simplest type of nontrivial

system. There are two dependent variables, the enthalpy u and a quantity $\bar{\chi}$ representing the fraction of material gasified at each point, but in fact in many cases $\bar{\chi}$ is an explicit algebraic function of u, in which case the problem can be put in Stefan-like form. Departures from this condition are characterized by the fact that $\bar{\chi}$ is constant in time. Accordingly, an analysis of the mathematical changes wrought by enlargement of the Stefan problem to the gasification problem may be very informative with respect to the phenomena to be expected when one deals with more general parabolic systems.

From the point of view of numerical analysis, there are two aspects of our treatment which may be of interest. The first is the means we use to deposit radiant energy on a moving, generally irregular, surface (the gas-solid interface) without explicitly tracking the surface. The second feature is that, in certain regimes of the initial and boundary data, the problem looks like a parabolic problem with fixed boundary and Neumann boundary data. In that regime our algorithm will solve the problem without explicitly locating the boundary. This is to be compared with limiting regimes in which the classical Stefan problem reduces to a parabolic problem with fixed boundary and Dirichlet data. Certain algorithms which have been given for the Stefan problem will solve this problem without explicitly locating the boundary [2, 1, 4].

2. Governing Assumptions

Typically in the gasification problem, we will assume that the heat conduction in the interior of the solid may be described by the equation

$$u_t = \Delta f(u) \ , \tag{2.1}$$

where we may think of u as the "enthalpy" per unit volume and $f(u)$ as the "temperature". $f(u)$ will be a nondecreasing Lipschitz-continuous function of u. We shall assume that the solid material will only gasify upon reaching a critical gasification temperature, which we may take equal to 0. Thus, (2.1) will hold in the region where the temperature is below this number, that is, is negative.

Suppose the energy transferred to the solid by the external energy source is F times a Dirac measure on the surface. When the temperature of the solid material at the surface remains below the gasification temperature, energy conservation at the solid boundary is expressed as

$$\frac{\partial}{\partial n} (f(u)) = F \ , \tag{2.2}$$

where n is the unit outward normal of the surface. In this case the boundary is not changing, since no gasification is taking place. The mathematical statement of this is that

$$V \cdot n = 0 \ , \tag{2.3}$$

where $V \cdot n$ is the normal velocity of the boundary. However, during gasification the temperature at the surface is just the gasification temperature

$$f(u) = 0 \ , \tag{2.4}$$

and the surface moves with the normal velocity

$$-\lambda \, V \cdot n = F - \frac{\partial}{\partial n} f(u) \tag{2.5}$$

where λ is the increase in enthalpy per unit volume attained by the solid upon its being converted to gas.

There is no loss of generality in choosing u for the solid to be 0 at the gasification temperature 0. Then for the gas $u = \lambda$. We may thus extend the function $f(u)$, so far defined for $u < 0$, to the interval $u \in [0,\lambda]$ by

$$f(u) = 0, \quad 0 \leq u \leq \lambda . \tag{2.6}$$

When the boundary conditions (2.4) and (2.5) apply, the problem looks very much like a one-phase Stefan problem with sources, and it is known that a more concise way of writing (2.1), (2.4), and (2.5) is in the form of a "conservation" law [1]

$$u_t = \Delta f(u) + \sigma(x,t) , \tag{2.7}$$

where (2.7) now holds over all space and f has been extended by (2.6). For our problem, σ has the form

$$\sigma(x,t) = F\delta_{\partial\{u<0\}} . \tag{2.8}$$

The form (2.7) can also be used as the basis for an efficient numerical solution of N-dimensional problems which avoids the need for following the moving boundary. (The matter of the explicit appearance of the boundary in the source term can be treated by a method to be described in the sequel.)

There are, however, some important limitations to the applicability of the formulation (2.7). The "one-phase" Stefan problem is really a two-phase problem for which heat conduction takes place in only one phase. The non-conducting phase (in this case, the "upper" one) acts passively as long as the region it occupies is increasing with time, but when the region occupied by the conducting phase increases anywhere, the non-conducting phase acts as a reservoir of either positive or negative (in this case, positive) energy. In the one-phase Stefan problem under the influence of external sources, the free boundary can move in either way. In the gasification problem, on the other hand, the gas, once it blows away, has no further influence on the solid and in particular the free boundary can move only one way, since the gas cannot

resolidify. Thus, although the formulation (2.7), in which the equation is extended to the non-conducting phase, is quite natural for the one-phase Stefan problem, in our problem the notion of a coexisting "gas phase" is a fiction.

Nevertheless, the fact that at times the gasification problem can be put in the form (2.7) and the numerical simplifications brought about by this possibility serve as an inducement for us to find an appropriate version of the problem in the spirit of (2.7). We have observed that the process of gasification is irreversible, so that $V \cdot n \leq 0$. Thus, we can summarize the boundary conditions (2.2)-(2.5) by noting that (2.5) holds in all cases, but that on portions of the boundary, for certain times, we have

$$V \cdot n \leq 0, \quad f(u) = 0 , \tag{2.9a}$$

whereas on the remaining portions of the boundary or for the remaining times,

$$V \cdot n = 0, \quad f(u) \leq 0 . \tag{2.9b}$$

From $V \cdot n \leq 0$, we get

$$\frac{\partial}{\partial n} f(u) \leq F , \tag{2.10}$$

which looks mathematically something like an "obstacle" condition on $\frac{\partial f}{\partial n}$. We note that the conditions (2.9a) are of Dirichlet type for f and the conditions (2.9b) are of Neumann type for f. Thus, generally we may expect a switching back and forth between Neumann and Dirichlet boundary conditions, and an alternate stopping and starting of the boundary motion.

Immediately we discern a lack of regularity for the solution of the gasification problem as opposed to the Stefan solution. For, in the case of the latter, the temperature $f(u)$ has been seen to be continuous [3]. But if we extend $f(u)$ to the region where there is no solid (and thus $u \equiv \lambda$) by the convention $f(u) \equiv 0$ there, we see that in the case of the Neumann conditions (2.9b), $f(u)$ is generally discontinuous. (In fact, this is true

no matter what value we choose for $f(\lambda)$.) In addition, because the solid, upon gasification, is replaced by a vacuum, which is a perfect thermal insulator, the gasification problem possesses instabilities with respect to the initial and boundary data which do not occur for the Stefan problem. For example, by changing the initial enthalpy to λ on a set of arbitrarily small measure, we can partition the solid into a collection of non-interacting regions, on the boundary of each of which the boundary conditions (2.9b) obtain. Then, invoking the lack of continuity of $f(u)$ under the influence of these boundary conditions which was just observed, we may construct solutions for which there is no uniform continuity of $f(u)$ as the measure of the set on which u has been set to λ goes to 0, and for which thermal contact between regions on different sides of the discontinuities of f has been prohibited. In like manner, by shifting very slightly the positions of the sources of external radiant energy and the directions in which they radiate, one may gasify all the material along certain rays and thermally insulate different parts of the solid from one another, thereby profoundly affecting the solution. And by allowing the radiation to arrive in sharp pulses rather than uniformly distributed over a small interval of time, one may increase the gasification of the material at the surface while minimizing the conduction of heat to the interior.

In our picture the gas has enthalpy $u = \lambda$ and is transparent to radiation, and hence there is no mechanism whereby u can exceed λ. For the Stefan problem, one can give meaning to a value of u in $(0,\lambda)$: it is that a volume fraction

$$\gamma(u) = \frac{1}{\lambda} \max(u,0) = \frac{u_+}{\lambda} \tag{2.11}$$

at a point has enthalpy λ and is gas, while the remainder is solid with enthalpy 0. Since values of u in $(0,\lambda)$ arise quite naturally when one solves the Stefan problem with sources, (2.7), we may expect a similar situation to develop when we try to cast the gasification problem in like form. However, the values permitted the enthalpy at the solid boundary are now not restricted to the set $\{\lambda,0\}$, but may belong to the set $\{\lambda,\bar{u} \leq 0\}$. Accordingly, if we denote the volume fraction at each point that corresponds to enthalpy λ by $\bar{\chi}$, so that $(1 - \bar{\chi})$ denotes the volume fraction of solid with enthalpy $\bar{u} \leq 0$, we get for the total enthalpy u of the combination,

$$u = \bar{u}(1 - \bar{\chi}) + \bar{\chi}\lambda \ , \tag{2.12a}$$

or

$$\bar{\chi} = \frac{u - \bar{u}}{\lambda - \bar{u}} \geq \chi(u) \ . \tag{2.12b}$$

Here we have proceeded as if the solid material had a common enthalpy $\bar{u}$ when $\bar{\chi} < 1$. We could envisage situations in which, in the region where $0 \leq \bar{\chi} < 1$, we had volume fractions α_i of solid material with enthalpies $u_i \leq 0$, each set thermally insulated from the others. Then we would have

$$\sum_i \alpha_i = 1 - \bar{\chi}, \ \sum_i \alpha_i u_i = (1 - \bar{\chi})\bar{u} \ . \tag{2.13}$$

However, if we consider the assignment of initial and boundary conditions and the gasification process itself as phenomena which are essentially subject to multi-dimensional stochastic spatial fluctuations, albeit minute ones, it appears that the compartmentalization of the solid material on a microscopic level into such components thermally isolated from each other would occur with probability 0, and we shall consider the solid material to have a single-valued enthalpy $\bar{u}$ and single-valued temperature $f(\bar{u})$.

From the foregoing considerations, we may derive equations for the time evolution of $\bar{\chi}$. If gasification is taking place we have $\bar{u} = 0$ and

$$\bar{\chi} = \chi(u), \quad \bar{\chi}_t = ((\chi(u))_t)_+ = \left(\left(\frac{u_+}{\lambda}\right)_t\right)_+ . \tag{2.14a}$$

But if gasification is not taking place, we have Neumann conditions at the solid boundary, $\bar{u} < 0$, and

$$\bar{\chi} > \chi(u), \quad \bar{\chi}_t = 0 . \tag{2.14b}$$

If $\bar{\chi}(x,0) = \chi(u(x,0))$ $\forall x$, we can use (2.14a,b) to find $\bar{\chi}(x,t)$ immediately in terms of u:

$$\bar{\chi}(x,t) = \sup_{0 \le t' \le t} \chi(u(x,t')) . \tag{2.15}$$

As regards the absorption of energy at the solid surface, as given by (2.8), we treat the gas as if it were completely transparent to the radiation. The absorption of radiation in a region where gas and solid are interspersed on a microscopic level should then be proportional, at each point, to $1 - \bar{\chi}$. Accordingly, if O denotes the location of the source of radiation, and we assume the source to be isotropic, a relevant quantity at any point P is the following integral:

$$d(P,O) = \int_P^O (1 - \bar{\chi}(Q))ds , \tag{2.16}$$

where the integral is taken over the straight line connecting P to O. We consider the solid to be completely opaque to the radiation, and this leads to the requirement that all the radiant energy be deposited at points P where $d(P,O)$ is as small as possible, subject only to the constraint that

$$u(x,t) < \lambda \quad \forall x,t . \tag{2.17}$$

We have presented the physical considerations which have motivated our treatment of the gasification problem. In the next section we will present an algorithm to solve a time-discretized version of the problem. This algorithm will be of a sort that has been introduced to solve problems of the type (2.7), [1]. We should note, however, that although we may resort at times in the sequel to pseudo-physical language to interpret the algorithm which we develop, the algorithm to be presented will have been crafted to solve precisely the problem whose physical and mathematical countenances have been so far explained. The algorithm should not necessarily be construed as describing also any physically realistic problems of a more general nature.

3. Time-Discretized Formulation

If the Lipschitz coefficient of $f(u)$, as given in (2.1), is $1/\beta$, a suitable numerical scheme to solve (2.7) with $\sigma \equiv 0$ is, with τ a time step and $u(n\tau)$ approximated by u^n [1],

$$u^{n+1} = u^n - \beta f(u^n) + S\left(\frac{\tau}{\beta}\right)(\beta f(u^n)) \ , \tag{3.1}$$

where

$$S(h) \equiv e^{h\Delta} \tag{3.2}$$

is simply the linear semi-group generated by the operator Δ. In the problem we treat here, we may regard $S(h)$ as Green's function for the heat equation in $\mathbf{R}^N$. It will be convenient below to write out $S(h)$ in this fashion explicitly:

$$(S(h)v)(x) = \int_{\mathbf{R}^N} S(h;x,x')v(x')dx' \ . \tag{3.3}$$

A pseudo-physical interpretation of (3.1) is that the equation

$$u_t = \frac{1}{\beta}\,\Delta(f\beta) \tag{3.4}$$

is an equation giving the evolution of u in terms of a diffusion of $\beta f(u)$, and that to find u^{n+1} we take u^n, subtract off $\beta f(u^n)$, which is to be diffused, and then add back $S(\frac{\tau}{\beta})(\beta f(u^n))$, the result of the diffusion.

If we are dealing with a problem for which (2.14a) applies $\forall x,t$ such that $0 < \chi < 1$, then in fact (3.1), supplemented by a term to represent the effect of the external heat sources, will satisfactorily describe the time evolution. However, in the more general case in which we may also have $\bar{\chi} > \chi(u)$ and Neumann conditions at the boundary, this algorithm clearly will not suffice.

In the first place, according to the pseudo-physical type of reasoning introduced above, the true measure of the "thermal energy" of the solid, per unit volume of solid, should be $\beta f(\bar{u})$ and not $\beta f(u)$, and the total amount

of such thermal energy, per unit volume, is $\beta f(\bar{u})(1 - \bar{\chi})$. Here, in accord with (2.12a),

$$\bar{u} = \frac{u - \bar{\chi}\lambda}{1 - \bar{\chi}} \tag{3.5}$$

when $\bar{\chi} < 1$. Accordingly, we would subtract out $\beta f(\bar{u})(1 - \bar{\chi})$, then add back $S(\frac{T}{\beta})[\beta f(\bar{u})(1 - \bar{\chi})]$. However, in diffusing the thermal energy $\beta f(\bar{u})(1 - \bar{\chi})$, we have transmitted energy to regions where a fraction $\bar{\chi}$ of the volume acts as a perfect insulator. Hence this portion of the diffused thermal energy should be subtracted out and returned to the point from whence it came. This means subtracting out $\bar{\chi}S(\frac{T}{\beta})[\beta f(\bar{u})(1 - \bar{\chi})]$ and then adding $\int_{\mathbf{R}^N} S(\frac{T}{\beta};x',x)\bar{\chi}(x')\beta f(\bar{u}(x))(1 - \bar{\chi}(x))dx'$. This final subtraction of a portion of the diffused thermal energy and return to its source is the part of the algorithm designed to conform to the insulating properties of the vacuum and to yield the solution of a Neumann problem at the appropriate places on the boundary. It is a direct generalization of the method of "images" used to solve Neumann problems at planar boundaries for the classical equations of mathematical physics. Putting these arguments together, for the case when Green's function is symmetric, as it is here,

$$S(h;x,x') = S(h;x',x) , \tag{3.6}$$

we are led to construct the function

$$\begin{aligned} u^n = u^n &- \beta f(\bar{u}^n)(1-\bar{\chi}^n) + S(\tfrac{T}{\beta})[\beta f(\bar{u}^n)(1-\bar{\chi}^n)] \\ &- \bar{\chi}^n S(\tfrac{T}{\beta})[\beta f(\bar{u}^n)(1-\bar{\chi}^n)] + \beta f(\bar{u}^n)(1-\bar{\chi}^n)S(\tfrac{T}{\beta})(\bar{\chi}^n) . \end{aligned} \tag{3.7}$$

If there were no external energy sources, we would set u^{n+1} equal to $\bar{u}^n$. In that case, on approximating $S(h)$ by the first two terms of its formal Taylor expansion,

$$S(h) \to 1 + h\Delta \ , \tag{3.8}$$

we would get from (3.7), as $\tau \to 0$,

$$u_t = (1-\bar{\chi})\Delta((1-\bar{\chi})f(\bar{u})) - (1-\bar{\chi})f(\bar{u})\Delta(1-\bar{\chi}) \ . \tag{3.9}$$

In fact, (3.9) may be given a pseudo-physical interpretation by noting that it can be derived, in the limit as the "mean free path" $\rho \to 0$, from the Boltzmann-like equation

$$\begin{aligned} u_t = \frac{A}{\rho^N}\{\int_{R^N} g\left(\frac{|x-x'|}{\rho}\right) f(\bar{u}(x'))(1-\bar{\chi}(x))(1-\bar{\chi}(x'))dx' \\ - f(\bar{u}(x))(1-\bar{\chi}(x)) \int_{R^N} g\left(\frac{|x-x'|}{\rho}\right)(1-\bar{\chi}(x'))dx'\}, \end{aligned} \tag{3.10}$$

where $\int_0^\infty g(r)dr = 1$, $g \geq 0$, and $A\rho^2 = 0(1)$ as $\rho \to 0$. Formally, (3.9) may also be written

$$u_t = \nabla \cdot ((1 - \bar{\chi})^2 \nabla f(\bar{u})) \ . \tag{3.11}$$

However, when $f(\bar{u})$ and $\bar{\chi}$ are discontinuous, as may be the case at a sharp solid-gas interface in the circumstance of Neumann conditions at the boundary, the meaning of (3.11) in a distributional sense is not clear.

In the general case we have to add the effect of the external energy sources to $\bar{u}^n$ in order to get u^{n+1}. Let us suppose that the incident energy F in (2.8) has the form

$$F(x,t) = \frac{\tilde{F}(t)}{\omega_{N-1}} \frac{|n \cdot (x(0) - x)|}{|x(0) - x|^N} \tag{3.12}$$

where $x(0)$ is the location of the source and $\omega_{N-1} = |\partial B_N|$, B_N the unit ball in N dimensions.

The energy deposited between times $n\tau$ and $(n+1)\tau$ may reasonably be approximated by $\tau\sigma(x,n\tau)$ when σ is continuous with respect to t. When σ has the form (2.8), this quantity has a singularity at the solid boundary. However, during the time τ that energy is deposited, it is also being conducted into the interior in the manner described by equation (2.1). Accordingly, if f_0' is a local value of $f'(u)$ in the solid and $f_0' > 0$, the energy will be spread out over a distance $O((\tau \ell n \frac{1}{\tau})^{1/2})$ after the time interval. It will be important for us to take this fact into account when depositing the incident radiant energy. To spread the energy out over a distance larger than $O((\tau \ell n \frac{1}{\tau})^{1/2})$ would be needlessly to increase the width of the free boundary (that is, the distance over which $\bar{\chi}$ changes from "near 0" to "near 1") generated by the algorithm. Experience with the Stefan problem leads us to expect an approximate free boundary of width $O((\tau \ell n \frac{1}{\tau})^{1/2})$, anyway [2]. Thus, we calculate u^{n+1} from the equation

$$u^{n+1}(x) = \tilde{u}^n(x) + \begin{cases} \dfrac{\sqrt{\tau}\,\tilde{F}(n\tau)(1-\bar{\chi}^n(x))}{\omega_{N-1}|x(0)-x|^{N-1}}, \\ \qquad 0 < d^n(x) < \sqrt{\tau} \\ 0 \qquad d^n(x) > \sqrt{\tau} \end{cases} \tag{3.13a}$$

where, from (2.16),

$$d^n(x) = \int_x^0 (1 - \bar{\chi}^n(Q))ds \ . \tag{3.13b}$$

Once u^{n+1} has been found, $\bar{\chi}^{n+1}$ is determined in accordance with a semi-discrete version of (2.15):

$$\bar{\chi}^{n+1} = \max(\bar{\chi}^n, \chi(u^{n+1})) \ . \tag{3.14}$$

If we refer to (2.12a) and (3.5), we find from (3.7) that

$$\frac{\tilde{u}^n - \lambda\bar{\chi}^n}{1 - \bar{\chi}^n} \leq 0 ,$$

and thus

$$\chi(\tilde{u}^n) \leq \bar{\chi}^n . \tag{3.15}$$

Accordingly, if there are no external energy sources and $u^{n+1} = \tilde{u}^n$, we get from (3.14) that $\bar{\chi}^{n+1} = \bar{\chi}^n$. This simply says that no material is gasified in the absence of external sources.

We have only to check that the algorithm (3.7), (3.13), (3.14) guarantees that, if $0 \leq \bar{\chi}^n \leq 1$, then the following two conditions are satisfied: (i) $0 \leq \bar{\chi}^{n+1} \leq 1$ and (ii) the time-discretized version of (2.17) holds, or $u^{n+1} \leq \lambda$. These two conditions are actually equivalent, by (2.11), (3.14), and the assumption $0 \leq \bar{\chi}^n \leq 1$. By direct calculation from (2.12a), (3.7), and (3.13), we get

$$u^{n+1} \leq \bar{\chi}^n\lambda + \frac{(1 - \bar{\chi}^n)\sqrt{\tau}\,\tilde{F}(n\tau)}{\omega_{N-1}|x(0) - x|^{N-1}} . \tag{3.16}$$

(3.16) will imply that $u^{n+1} \leq \lambda$ if we impose the following stability condition on the size of the time step τ:

$$\tilde{F}(n\tau)\sqrt{\tau} \leq \lambda\omega_{N-1}[\mathrm{dist}(0,\{x|u(x,0) < \lambda\})]^{N-1} . \tag{3.17}$$

The sufficiency of (3.17) follows from the observation that, if $\bar{\chi}^n(x) < 1$, then $\bar{\chi}^0(x) < 1$ and $|x(0) - x| \geq \mathrm{dist}(0,\{x|u(x,0) < \lambda\})$. In the calculations to be described in the next section, we impose the stability condition (3.17) on τ.

4. Numerical Quadrature and Computational Results

The computations we have actually performed have been one-dimensional calculations for the case

$$\lambda = 1, \; f(u) = \min(u,0) \; . \tag{4.1}$$

We see from (4.1) that we can choose $\beta = 1$. The algorithm described in the last section can now be written

$$u^{n+1} = u^n + (1-\bar{\chi}^n)[(S(\tau)-1)(1-\bar{\chi}^n)f(\bar{u}^n) + f(\bar{u}^n)(S(\tau)-1)\bar{\chi}^n]$$

$$+ \begin{cases} \dfrac{\tilde{F}(n\tau)}{2}\sqrt{\tau}\,(1-\bar{\chi}^n) & 0 < d^n < \sqrt{\tau} \\ 0 & d^n > \sqrt{\tau} \end{cases} , \tag{4.2a}$$

$$\bar{\chi}^{n+1} = \max(\bar{\chi}^n, \chi(u^{n+1})) \; . \tag{4.2b}$$

Since the expression (3.5) for $\bar{u}$ becomes indeterminate when $\bar{\chi} \to 1$, we have used the following determinaton of $(1-\bar{\chi})f(\bar{u})$ that is well-defined for all values of $\bar{\chi} \in [0,1]$:

$$(1-\bar{\chi})f(\bar{u}) = \min(u-\bar{\chi},0) \; . \tag{4.3}$$

We have broken the spatial region into a finite number of cells I_i of width Δx_i, $1 \le i \le I$. We have imposed the conditions $\bar{\chi} = 0$, $f(\bar{u}) = -1$ at the left and $\bar{\chi} = 1$ at the right, and we have considered the source to be at the right of the mesh. We denote the characteristic function of I_i by χ_i:

$$\chi_i(x) = \begin{cases} 1 & x \in I_i \\ 0 & x \in I_i \end{cases} , \tag{4.4}$$

we approximate the functions $u^n(x)$ and $\bar{\chi}^n(x)$ by the piecewise-constant functions

$$u^n \sim \sum_{i=1}^{I} u_i^n \chi_i \ , \tag{4.5a}$$

$$\bar{\chi}^n \sim \sum_{i=1}^{I} \bar{\chi}_i^n \chi_i \ , \tag{4.5b}$$

and we denote the total energy in I_i by U_i^n:

$$U_i^n = (\Delta x_i) u_i^n \ . \tag{4.6}$$

For the operator $S(\tau)$, we have used an explicit finite-difference scheme. Then the operator can be represented by its effect on a characteristic function:

$$S(\tau)\chi_i = \frac{\Delta x_i}{\Delta x_{i-1}} c_i^- \chi_{i-1} + c_i^0 \chi_i + \frac{\Delta x_i}{\Delta x_{i+1}} c_i^+ \chi_{i+1} \ . \tag{4.7}$$

Suitable coefficients c_i^-, c_i^0, c_i^+ can easily be calculated, and we note only the result of such a calculation [6, p. 29]:

$$c_i^- = 3\tau[\Delta x_{i-\frac{1}{2}}(\Delta x_{i-1}+\Delta x_i+\Delta x_{i+1})]^{-1} \ , \tag{4.8a}$$

$$c_i^+ = 3\tau[\Delta x_{i+\frac{1}{2}}(\Delta x_{i-1}+\Delta x_i+\Delta x_{i+1})]^{-1} \ , \tag{4.8b}$$

$$c_i^0 = 1 - c_i^- - c_i^+ \ . \tag{4.8c}$$

Here we have set

$$\Delta x_{i+\frac{1}{2}} = \frac{1}{2}(\Delta x_i + \Delta x_{i+1}) \tag{4.9a}$$

and

$$\Delta x_0 = \Delta x_1, \quad \Delta x_{I+1} = \Delta x_I \ . \tag{4.9b}$$

We recall that the operator $S(\tau)$ is symmetric, as stated in (3.6). However, the finite-difference analog of $S(\tau)$ given above is not necessarily symmetric if the mesh widths Δx_i vary with i. This lack of symmetry could

lead to a departure from strict energy conservation if one were to use the algorithm (4.2) unthinkingly. Such a departure can be avoided if we return to the argument given in the paragraph immediately preceding (3.6). What we should do is use the finite-difference representation of $S(\tau)$ given above when $S(\tau)$ operates on $(1 - \bar{\chi}^n)f(\bar{u}^n)$, and use the transpose of this representation when $S(\tau)$ operates on $\bar{\chi}^n$. The transpose of the finite-difference representation is given by

$$S^T(\tau)\chi_i = c_{i-1}^{+}\chi_{i-1} + c_i^0\chi_i + c_{i+1}^{-}\chi_{i+1} . \tag{4.10}$$

The explicit nature of our representation of $S(\tau)$ forces on us an additional stability condition for τ. A sufficient condition is that τ satisfy

$$\tau \leq \frac{1}{2} \min_i((\Delta x_i)^2) . \tag{4.11}$$

The finite-difference treatment of the energy deposition from outside apportions to the cell I_i the amount of energy V_i^n, given by

$$V_I^n = \min\left(\frac{\tilde{F}(n\tau)\tau}{2}, (1-\bar{\chi}_I^n)\Delta x_I\sqrt{\tau}\,\frac{\tilde{F}(n\tau)}{2}\right) , \tag{4.12a}$$

$$V_i^n = \left(\min\left(\frac{\tilde{F}(n\tau)}{2}\,\tau - \sum_{j=i+1}^{I} V_j^n, (1-\bar{\chi}_i^n)\Delta x_i\sqrt{\tau}\,\frac{\tilde{F}(n\tau)}{2}\right)\right)_+ , \tag{4.12b}$$

$$1 \leq i \leq I - 1 .$$

Denoting

$$Y_i^n \equiv \min(u_i^n - \bar{\chi}_i^n, 0) \tag{4.13}$$

and putting the expressions above together, we find, for $2 \leq i \leq I - 1$,

$$U_i^{n+1} = U_i^n + (1-\bar{\chi}_i^n)[Y_{i+1}^n c_{i+1}^- \Delta x_{i+1} + Y_{i-1}^n c_{i-1}^+ \Delta x_{i-1}]$$

$$- Y_i^n \Delta x_i [(1-\bar{\chi}_{i+1}^n) c_i^+ + (1-\bar{\chi}_{i-1}^n) c_i^-] + V_i^n \ . \tag{4.14}$$

Special expressions are needed for $i = 1$ and $i = I$. Since we are imposing the conditions $\bar{\chi} = 0$ and $f(\bar{u}) = -1$ at the left and $\bar{\chi} = 1$ at the right, we set

$$\bar{\chi}_0^n = 0, \ \bar{\chi}_{I+1}^n = 1, \ Y_0^n = -1, \ Y_{I+1}^n = 0 \ . \tag{4.15}$$

Thus we get for $i = 1$

$$U_1^{n+1} = U_1^n + (1-\bar{\chi}_1^n)(Y_2^n c_2^- \Delta x_2 - c_0^+ \Delta x_1) - Y_1^n \Delta x_1 [(1-\bar{\chi}_2^n) c_1^+ + c_1^-] + V_1^n \ , \tag{4.16a}$$

where

$$c_0^+ = \frac{3\tau}{\Delta x_1 (2\Delta x_1 + \Delta x_2)} \ , \tag{4.16b}$$

and for $i = I$

$$U_I^{n+1} = U_I^n + (1-\bar{\chi}_I^n) Y_{I-1}^n c_{I-1}^+ \Delta x_{I-1} - Y_I^n \Delta x_I (1-\bar{\chi}_{I-1}^n) c_I^- + V_I^n \ . \tag{4.16c}$$

The computational loop is completed by setting

$$u_i^{n+1} = U_i^{n+1} / \Delta x_i \tag{4.17a}$$

and

$$\bar{\chi}_i^{n+1} = \max((u_i^{n+1})_+, \bar{\chi}_i^n) \ . \tag{4.17b}$$

In the more general one-dimensional case, we get a finite-difference relation of the sort

$$
\begin{aligned}
U_i^{n+1} = U_i^n &- \beta(1-\bar{\chi}_i^n) f(\bar{u}_i^n)\Delta x_i \\
&+ (1-\bar{\chi}_i^n)\{\Delta x_{i+1} c_{i+1}^- f(\bar{u}_{i+1}^n)(1-\bar{\chi}_{i+1}^n) \\
&+ \Delta x_{i-1} c_{i-1}^+ f(\bar{u}_{i-1}^n)(1-\bar{\chi}_{i-1}^n) \\
&+ \Delta x_i c_i^0 f(\bar{u}_i^n)(1-\bar{\chi}_i^n)\} \\
&+ f(\bar{u}_i^n)(1-\bar{\chi}_i^n)\Delta x_i (c_i^{+-n}\chi_{i+1} \\
&+ c_i^{0-n}\chi_i + c_i^{--n}\chi_{i-1}) + V_i^n
\end{aligned}
\tag{4.18}
$$

where c_i^+ and c_i^- are as given in (4.8a,b), and

$$c_i^0 = \beta - c_i^- - c_i^+ . \tag{4.19}$$

A sufficient condition for stability of the finite-difference scheme is

$$\tau \leq \frac{1}{2}\beta \min_i(\Delta x_i)^2 . \tag{4.20}$$

$\bar{u}_i^n$ is given in terms of u_i^n and $\bar{\chi}_i^n$ by means of (3.5). For computational reasons, for a sufficiently small ε, one may wish to calculate $\bar{u}_i^n$ from

$$\bar{u}_i^n = \begin{cases} \dfrac{u_i^n - \lambda\bar{\chi}_i^n}{1 - \bar{\chi}_i^n} & 1 - \bar{\chi}_i^n > \varepsilon \\ 0 & 1 - \bar{\chi}_i^n \leq \varepsilon \end{cases} . \tag{4.21}$$

We performed a calculation with $I = 120$, $\Delta x_i = .01$ $\forall i$, $\tau = .00005$, $u_i^0 = -1$, $1 \leq i \leq 100$, $u_i^0 = 1$, $101 \leq i \leq 120$, and $\bar{\chi}_i^0 = \chi(u_i^0)$. We chose $F(t) = 6$ independent of t.

Letting the intersection of I_{100} and I_{101} be located at $x = 0$ and denoting by the "exact solution" the solution of the gasification problem posed on $\mathbf{R}$ with the solid region initially occupying $\mathbf{R}_-$ and $u(x,0) = -1$ $\forall x \in \mathbf{R}_-$, we find that initially the exact solution satisfies

Neumann conditions at $x = 0$, and that $u(0,t)$ is given by $-1 + 6\sqrt{t/\pi}$, until the time $t_0 = \pi/36$, when gasification commences and the front begins to move. Further analysis of the exact solution indicates that for $t > t_0$ but $t - t_0$ small, the position of the front is at

$$\Sigma(t) = -\frac{54}{\pi^2}(t - t_0)^2 .$$

If the solution of the gasification problem has a self-similar behavior as $t \to \infty$, it will be of the form

$$u \to -1 + e^{\frac{3}{2}x + \frac{9}{4}(t-t_1)} \quad \text{for} \quad x < -\frac{3}{2}(t - t_1) .$$

The problem was run to time $t = .3$. The following table gives the computed position $\Sigma(t)$ of the free boundary, defined to be the point where $\bar{\chi} = .5$ and determined by linearly interpolating values of $\bar{\chi}$ between adjacent cells such that $\bar{\chi} - .5$ changes sign from one to the other. In all cases the front was never spread out over more than one or two computational cells.

TABLE 4.1

Computed Position $\Sigma(t)$ of Free Boundary

t	$\Sigma(t)$	t	$\Sigma(t)$
.09	0	.20	-.098
.10	-.005	.21	-.109
.11	-.010	.22	-.119
.12	-.019	.23	-.130
.13	-.028	.24	-.142
.14	-.037	.25	-.154
.15	-.046	.26	-.166
.16	-.055	.27	-.177
.17	-.064	.28	-.189
.18	-.076	.29	-.200
.19	-.087	.30	-.212

In order to test that the algorithm described here does indeed predict the cessation of gasification, cooling off of the solid surface, and resumption of Neumann conditions at the boundary under the appropriate circumstances, for $n\tau > .3$ we set $U_{61}^{n} = 0$. As expected, the motion of the free boundary soon ceased, and the steady state value of the position was computed as $\Sigma = -.216$. The solution between $i = 61$ and the free boundary reached a steady state u with the slope $u_x = 3$, as it should, from (2.2) and (3.12).

5. Remarks on Monotonicity

We would like to conclude this paper with some suggestions regarding the sorts of monotonicity properties we might expect for the solution. It is well known, of course, that the solution of the Stefan problem depends monotonically on the initial and boundary data, and also on the external sources. In the case when $\bar{\chi} = \chi(u)$ $\forall x,t$, then we also have such monotone dependence. For, we are then dealing with the situation in which the gasification front is moving and $f(u) = 0$ at the free boundary. In this event, (3.11) is meaningful in a distributional sense and may be rewritten as

$$u_t = \Delta\theta(u) \tag{5.1a}$$

for an appropriate function θ:

$$\theta'(u) = (1 - \chi(u))^2 f'(u) \ . \tag{5.1b}$$

But (5.1a) is in the same form as the Stefan problem, and the monotonicity follows in the usual way.

In general, we can show that this type of monotonicity does not hold for the gasification problem. Consider a problem with $f(u) = \min(u,0)$ and $\lambda = 1$, and with the boundary condition $(f(u))_x \neq 0$ imposed at $x = 0$. Suppose the initial data are $u(x,0) = -1$ for $0 < x < 1$, $u(x,0) = 0$ for $1 < x < 2$, and $u(x,0) = 1$ for $x > 2$. If we do not irradiate the boundary of the solid, at $x = 2$, with energy, the problem will evolve as a diffusion process in $0 < x < 2$ with homogeneous Neumann data at $x = 2$. Eventually the steady state $u(x) = -\frac{1}{2}$ for $0 < x < 2$, $u(x) = 1$ for $x > 2$ will be achieved. On the other hand, suppose we irradiate the solid with $\frac{\tilde{F}(t)}{2} = \frac{1}{\delta}$ for $0 < t < \delta$ and $\tilde{F}(t) = 0$ for $t > \delta$. As we let $\delta \to 0$, we find that any diffusion of thermal energy in the region occupied by the solid in the time interval $0 < t < \delta$ becomes negligible. Then, in the limit as $\delta \to 0$, we have for $u(x,\delta)$ the following values: $u(x,\delta) = -1$ for $0 < x < 1$,

$u(x,\delta) = 1$ for $x > 1$. This is also the steady state achieved for the problem. Thus, by irradiating the solid surface with energy, we have actually reduced the steady state values of u in portions of the interior.

A tempting conjecture to make is that, if we have two solutions $u_1^n(x)$, $\bar{\chi}_1^n(x)$ and $u_2^n(x)$, $\bar{\chi}_2^n(x)$ of the gasification algorithm, subjected to the same boundary conditions and external energy source located at a point with x-coordinate equal to X, then if $u_1^n(x,y) \geq u_2^n(x,y) \forall x,y$ and $\bar{\chi}_1^n(x,y) = \bar{\chi}_2^n(x,y) \forall x,y$, it will follow, for any $p \geq 0$, that

$$\int_{\mathbf{R}^{N-1}} \int_{X-\xi}^{X+\xi} u_1^{n+p}(x,y)\,dxdy \geq \int_{\mathbf{R}^{N-1}} \int_{X-\xi}^{X+\xi} u_2^{n+p}(x,y)\,dxdy$$

and

$$\int_{\mathbf{R}^{N-1}} \int_{X-\xi}^{X+\xi} \bar{\chi}_1^{n+p}(x,y)\,dxdy \geq \int_{\mathbf{R}^{N-1}} \int_{X-\xi}^{X+\xi} \bar{\chi}_2^{n+p}(x,y)\,dxdy$$

for all $\xi \in \mathbf{R}_+$. Here y merely labels the $N - 1$ coordinates of a point in a hyperplane orthogonal to the x-axis. If the conjecture is true, we will get monotonicity properties for Radon transforms of the energy distributions. However, at this point we do not have any solid indications regarding the accuracy of the conjecture.

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REFERENCES

[1]. Berger, A.E., Brezis, H., and Rogers, J.C.W.: A Numerical Method for Solving the Problem $u_t - \Delta f(u) = 0$. R.A.I.R.O., Analyse Numerique (1979).

[2]. Berger, A.E., Ciment, M., and Rogers, J.C.W.: The Alternating Phase Truncation Method for Numerical Solution of a Stefan Problem. SIAM J. Numer. Anal. (1979).

[3]. Caffarelli, L.A. and Evans, L.C.: Continuity of the Temperature in the Two Phase Stefan Problem, to appear.

[4]. Chorin, A.J., Hughes, T.J.R., McCracken, M.F., and Marsden, J.E.: Product Formulas and Numerical Algorithms. Comm. Pure Appl. Math. 31(1978), 205.

[5]. Rogers, J.C.W.: The Formulation of Selected Free Boundary Problems as Conservation Laws, Proceedings of Intensive Seminar on Free Boundary Problems, Pavia (1979).

[6]. Rogers, J.C.W. and Favin, S.: Computation of Water Waves. The Johns Hopkins University Applied Physics Laboratory TG1325 (1979).

[7]. Sekerka, R.F.: Morphological Stability, Crystal Growth, an Introduction. P. Hartman, North-Holland 1973.

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A problem of gasification and heating of a solid due to the action of an external energy source is discussed. The problem involves a moving boundary when the solid gasifies. At parts of the boundary where gasification is taking place, a model problem looks very much like the one-phase Stefan problem with an energy source at the moving boundary. However, any gas produced is assumed

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20. ABSTRACT - Cont'd.

to blow away immediately, and there is no conduction to the solid from the outside, even when the surface temperature of the solid is below the gasification temperature. Accordingly, if the temperature is extended to a function defined over all space by setting it equal to the gasification temperature outside, the temperature will not necessarily be continuous at the boundary, and instead a Neumann condition may be satisfied there. Also, no resolidification is possible, so that the region occupied by the solid cannot increase. Thus, one has the possibility of a situation in which the boundary may alternately move and be stationary. A generalized formulation of the problem is given, a numerical algorithm is described, and computational results are presented.


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